Analysis of collagen structure in parchment by Small angle X-ray diffraction

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Parchment has the characteristic molecular packing associated with other collagen rich structures, particularly skin. A wealth of information is available about the structure of collagen and its hierarchical arrangements from the molecular structure to the organisation of fibres in a tissue. X-ray diffraction of collagen has provided information about the molecular organisation of individual collagen molecules and the way that they pack together to form fibrils.

The main consideration with understanding the structure of parchment at the molecular level is that the collagen within parchment has undergone deterioration due to external factors. It is important to assess this deterioration for the conservation of historically important documents. Collagen deterioration at the molecular level corresponds to the breakage of covalent bonds and a subsequent increase in molecular disorder. With increasing molecular disorder the hierarchical organisation of collagen, from the molecular to the mesoscopic levels (Figure 1), is compromised.

Small angle X-ray diffraction provides a means of monitoring changes in the physical organisation of the collagen within the parchment sample. With increasing disorder, the characteristic pattern of collagen from parchment changes and displays less of an organised structure.

Principal Components Analysis (PCA) is a statistical technique that is capable of describing the nature and degree of variance in a data set. PCA of linear profiles of X-ray diffraction patterns (Figure 2) is capable of describing changes in the linear traces such as variations in the levels of diffuse scatter, the presence or absence of collagen or lipids, the crystallinity of the samples and changes in the periodicity of the collagen arrangement. This allows for a more detailed and quantifiable analysis of discrete changes occurring within parchment that can be detected by X-ray diffraction (Figure 3).

By using X-ray diffraction and PCA, subtle changes brought about in parchment, for instance gelatinisation and alterations in the structural organisation of collagen, can be analysed. External factors that may contribute to parchment deterioration include short-term factors such as fire, flood or conservation techniques and longer-term factors such as humidity and pollution levels. The effect of these factors can subsequently be stated in terms of damage assessment of parchment.

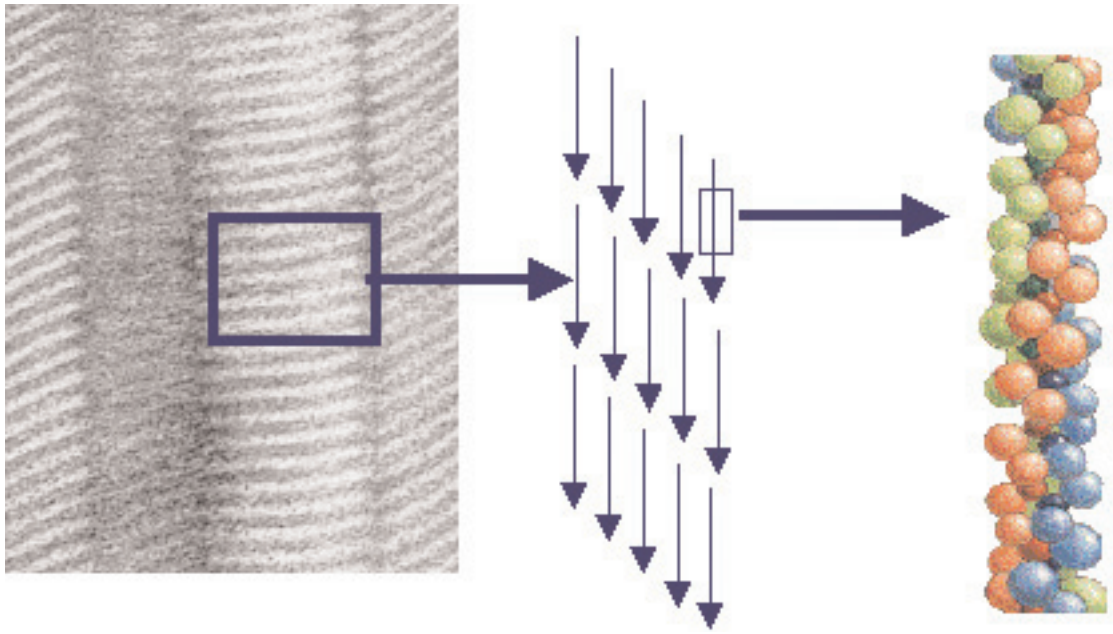

Figure 1. The hierarchical arrangement of collagen from parchment. (a)Transmission Electron Microscope image of collagen. The banding pattern is characteristic of the repeating gap/overlap function of collagen, which has a 67 nm axial repeat or D-period. This exists at the mesoscopic level. (b) Representation of the quarter-staggered arrangement of collagen molecules within a fibril at the nanoscopic level. (c) Diagram of the collagen triple helix; this exists at the molecular level, where the sidegroups of individual amino acids are shown as spheres..

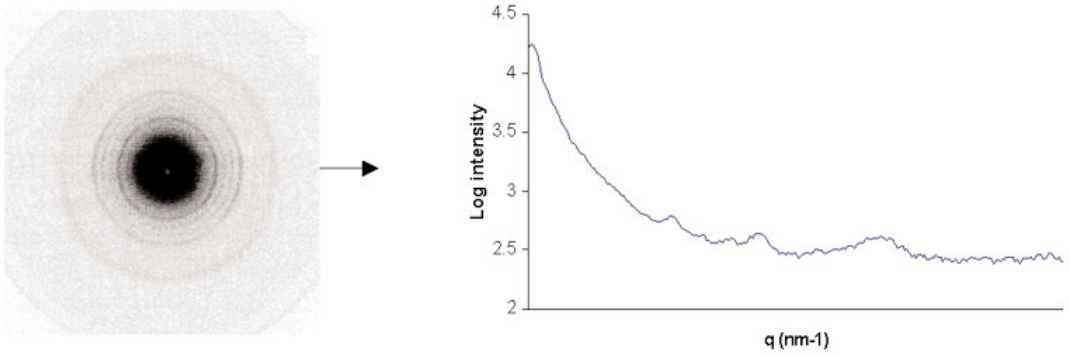

Figure 2. Small angle X-ray diffraction pattern from parchment sample USH01 and the linear profile of its radial integration. Discernible are the 6th, 7th, 8th and 9th orders of the collagen D-period and also the lipid ring.

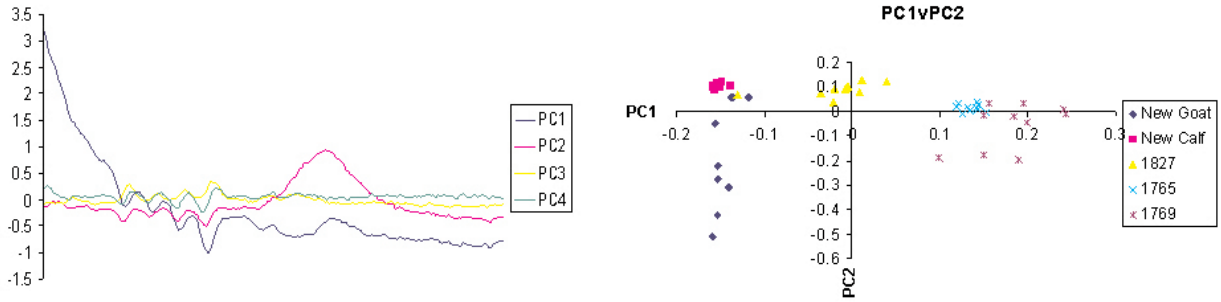

Figure 3. Principal components analysis results from a data set of forty linear traces from five different parchment samples. (a) The principal components. These four components account for over 97% of the variance in the data set. PC1 can be interpreted as variations in the diffuse scatter in the samples. PC2 accounts for the lipid ring. PC3 and PC4 display minor changes in the collagen D-period. (b) The correlation coefficients of the original data to the principal components 1 and 2. If the original data shows positive correlations to the principal components then the features of the principal components are present; if the correlation is zero then the feature is not present; if the correlation is negative then the feature is the reverse of the component. There is a clear grouping of the samples in the correlation coefficient scatter plot.